Transport Equations for CAD Modeling of $Al_xGa_{1-x}N/GaN$ HEMTs

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Abstract

HEMTs formed from $Al_xGa_{1-x}N/GaN$ heterostructures are being investigated for high RF

power and efficiency around the world by many groups, both academic and industrial. In these

devices, the 2DEG formation is dominated by both spontaneous and piezoelectric polarization

fields, with each component having nearly the same order of magnitude. The piezoelectric

portion is induced by the mechanical strain in the structure, and to analyze these devices, one

must incorporate the stress/strain relationships, along with the standard semiconductor transport

equations. These equations for Wurtzite GaN are not easily found in the open literature, hence

this paper summarizes them, along with the constitutive equations for piezoelectric materials.

The equations are cast into the format for the Wurtzite crystal class, which is the most common

way GaN is grown epitaxially.

1. Introduction

The HEMTs fabricated from wide bandgap semiconductors (WBGS) such as

$Al_xGa_{1-x}N/GaN$ outperform HEMTs based on III-V semiconductors by a factor of nearly 10 in

microwave power density. The power added efficiency (PAE) has been reported to be in the

range of 30 to 40 percent [1]. These heterostructure field effect transistors formed from

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$Al_xGa_{1-x}N$/GaN layers have high 2DEG densities primarily due to spontaneous and piezoelectric polarization fields inherent in this material system. At this time the devices have not performed as well as theory predicts, and there are several reasons for that. One is the problem of trapped charge in undesired locations due to crystal imperfections which cause both current collapse and knee walk-out. Another is the strong self-heating effect. A third is leakage. These problems are a strong function of the charge distribution; and if one desires an accurate analysis for this distribution for a given structure, the stress or strain should be considered at all points, which up until now has not been done. Recent studies concerning the phenomenon of current collapse have indicated the need to consider the piezoelectric effect in detail, and the subsequent carrier confinement in the gate-drain access area [2–4]. In general then, to model the electrical characteristics of the HEMT accurately, one must solve simultaneously the equations of stress and strain, Poisson's, and Schroedinger's equations. To that one appends the thermal generation (crystal heating due to the carriers) portion in a given simulator. This is needed as the self-heating in these devices is significant. Figure 1 summarizes the above discussions. The ideal and the often measured I_D-V_D characteristics are shown to indicate the knee walk-out, incomplete pinch-off at large V_D, and perhaps some breakdown current. The conceptual flowchart indicates the need to solve several sets of equations. Materials with negligible piezoelectric effect would not require the two left boxes; those for mechanical strain and the piezoelectric constitutive equations. To the best of our knowledge, we have not come across all of these equations as they pertain to the $Al_xGa_{1-x}N$/GaN material system; and hence this paper presents them for the first time. They are intended to serve as a guide for CAD modeling of $Al_xGa_{1-x}N$/GaN HEMTs.

2. Analysis

Figure 2 is a cartoon that depicts a double recessed channel HEMT. The assumed contours of constant strain or stress are given at corners and at edges of contact pads and the gate. The mechanical equations of equilibrium [5] for any arbitrary material in the presence of an electric field are shown below. We assume an x, y, z coordinate system and the positive z-axis points from the GaN buffer into the $Al_xGa_{1-x}N$ epitaxial layer.

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial T_{yx}}{\partial y} + \frac{\partial T_{zx}}{\partial z} - qn\frac{\partial \phi}{\partial x} = 0 \tag{1a}$$

$$\frac{\partial T_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial T_{zy}}{\partial z} - qn\frac{\partial \phi}{\partial y} = 0 \tag{1b}$$

$$\frac{\partial T_{xz}}{\partial x} + \frac{\partial T_{yx}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} - qn\frac{\partial \phi}{\partial z} = 0 \tag{1c}$$

where σ_{ii} and T_{ij} are components of stress and q, n, ϕ are the electronic charge, carrier density and electrostatic potential, respectively. The last terms are components of the body force, which we assume is the charge density times the electric field component. Assume the constitutive equations for piezoelectric dielectrics are applicable to a semiconductor; then following [6] the piezoelectric strain equations are

$$\overleftrightarrow{S} = d_T \cdot \overline{E} + s^E : \overleftrightarrow{T} \tag{2a}$$

$$\overline{D} = \epsilon_0 \, \kappa^T \cdot \overline{E} + d : \overleftrightarrow{T} \tag{2b}$$

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where $\vec{S}, d_T, \overline{E}, s^E, \overline{D}, \in_0, \kappa^T$, are the strain, piezoelectric strain components, electric field, compliance constants, electric flux density, free space dielectric constant, and relative dielectric constant, respectively. Alternatively one may use the piezoelectric stress equations

$$\ddot{T} = -e : \overline{E} + c^E : \vec{S} \tag{3a}$$

$$\overline{D} = \in_0 \kappa^S \cdot \overline{E} + e : \ddot{S} \tag{3b}$$

where $\ddot{T}$, e, and c^E are the stress, piezoelectric stress constants, and stiffness constants, respectively. Since GaN is grown primarily in the Wurtzite crystal class, equations (3a) and (3b) simplify to the following form [7]:

$$
\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ T_{yz} \\ T_{zx} \\ T_{xy} \end{bmatrix}
=
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\
c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{c_{11}-c_{12}}{2}
\end{bmatrix}
\begin{bmatrix} \in_{xx} \\ \in_{yy} \\ \in_{zz} \\ \gamma_{yz} \\ \gamma_{zx} \\ \gamma_{xy} \end{bmatrix}
-
\begin{bmatrix}
0 & 0 & e_{31} \\
0 & 0 & e_{31} \\
0 & 0 & e_{33} \\
0 & e_{15} & 0 \\
e_{15} & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}
\tag{4a}
$$

$$
\begin{bmatrix} D_x \\ D_y \\ D_z \end{bmatrix}
= \in_0
\begin{bmatrix}
\kappa_{11} & 0 & 0 \\
0 & \kappa_{11} & 0 \\
0 & 0 & \kappa_{33}
\end{bmatrix}
\begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}
+
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & e_{15} & 0 & 0 \\
e_{31} & e_{31} & e_{33} & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix} \in_{xx} \\ \in_{yy} \\ \in_{zz} \\ \gamma_{yz} \\ \gamma_{zx} \\ \gamma_{xy} \end{bmatrix}
\tag{4b}
$$

To this we include the compatibility expressions

$$\frac{\partial u}{\partial x} = \epsilon_{xx}, \frac{\partial v}{\partial y} = \epsilon_{yy}, \frac{\partial w}{\partial z} = \epsilon_{zz}$$

$$\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} = \gamma_{yz}, \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} = \gamma_{zx}, \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = \gamma_{xy}$$

(5)

Where u, v, w, are the material displacements. Finally we add the static relationships

$$\overline{E} = -\nabla\phi, \ \nabla \cdot \overline{J}_n = 0, \ \nabla \cdot \overline{D} = q\left(N_D^+ + N_t^+ - n\right)$$

(6)

Where N_D^+, N_t^+, n are the doping, trap, and carrier concentrations, (holes are omitted for

brevity). Observe there are 20 equations in 20 unknowns; therefore, use of appropriate

mechanical and electrical boundary conditions will yield complete solutions. In principle, the

above would be solved along with the Poisson-Schroedinger, and heat generation equations in a

simulator. Further refinements can be made by including the deformation potentials that relate

bandgap to strain.

3. Discussion

There is considerable dispersion in the literature for the mechanical c_{ij} and s_{ij}, and

electrical constants e_i, d_j for GaN and AlN; so tables 1 to 4 are given for initial estimates, which

are based on averages from the literature.

The electric polarization due to the piezoelectric effect is recognized as either

$$\bar{P} = e : \ddot{S}$$

$$\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \in_{xx} \\ \in_{yy} \\ \in_{zz} \\ \gamma_{yz} \\ \gamma_{zx} \\ \gamma_{xy} \end{bmatrix} \qquad (7)$$

or

$$\bar{P} = d : \ddot{T}$$

$$\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ T_{yz} \\ T_{zx} \\ T_{xy} \end{bmatrix} \qquad (8)$$

Whereas the spontaneous polarization is assumed to appear only at the $Al_xGa_{1-x}N/GaN$ interface

[8]. In this treatment we have assumed the coordinate axes are such that the positive z-axis points

from the GaN buffer into the $Al_xGa_{1-x}N$ epitaxial layer. It is oriented along the (0001) direction

(the c-axis). The GaN is assumed to have a gallium face at the interface. The spontaneous

polarization is approximately -5.1×10^{-2} C/m $(\bar{a}_z)$ where $\bar{a}_z$ is the unit vector. More

information concerning the spontaneous polarization may be found in [9–10].

Most commercial solvers ignore equations (4) and (5), and thereby have solutions with restricted accuracy. We have included these equations into a solver which is at present undergoing beta-test before commercial release.

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Figure Captions

Figure 1: Flow chart to show where the mechanical stress/strain and piezoelectric constitutive equations fit into the calculation for charge distribution and carrier transport in a simulator. The lower portion depicts a general I_D-V_D drain characteristic indicating the problems of incomplete pinch-off, knee walk-out, and breakdown.

Figure 2: Schematic of a hypothetical GaN HEMT indicating stress/strain fields due to heterojunctions and metal pads. Shown are idealized stress/strain contours near the edges of metal contacts and steps. The AlN layer is shown to be in compression in the plane and tension normal to the plane.

Table 1: Average stiffness constants for GaN and AlN

C_{ij} (GPa)	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}
GaN	370	145	110	390	90
AlN	410	140	100	390	120

Table 2: Average compliance constants for GaN and AlN

$s_{ij} \left(\dfrac{m^2}{N} \times 10^{-12} \right)$	s_{11}	s_{12}	s_{13}	s_{33}	s_{44}
GaN	3.175	−1.044	−0.581	2.887	9.709
AlN	3.532	−1.014	−0.765	2.997	8.474

Table 3: Average Piezoelectric stress constants
for GaN and AlN

$e_{ij}\ \left(C/m^2 \right)$	e_{15}	e_{31}	e_{33}
GaN	−0.28	−0.35	+0.71
AlN	--	−0.6	+1.5

Table 4: Average piezoelectric strain constants
for GaN and AlN

$d_{ij}\ \left(10^{-10}\,cm/V\right)$	d_{15}	d_{31}	d_{33}
GaN	–2.75	–1.16	+2.39
AlN	–3.4	–2.65	+5.53